My toolbox presentation was on my research in SPRING Lab. I am working closely with PhD candidate Ji Tae Park. SPRING Lab is a biophysics lab that conducts research on oncology. The main treatment being studied is most applicable to ovarian cancer. The treatment involves a photosensitizer drug that is linked to an antibody. As the antibody-drug conjugate (ADC) diffuses out of the bloodstream, the drug is released into tumor cells. A laser is then applied to the tumor, activating the drug and killing the tumor cells. The goal of the treatment is to eliminate tumor cells with minimal side effects.

I am working on simulating the drug distribution through the tumor as a function of time in Python. To initialize the system, we used a **100 × 100 × 100** voxel grid and set initial drug concentrations in different areas. The system then evolves according to a set of differential equations using a forward Euler method. In the future, it would be beneficial to explore other numerical methods, such as the Verlet or Runge-Kutta methods.

So far, I have developed five versions of the simulation. The first two allowed only one drug molecule to be conjugated to each antibody—one with a single capillary through the center of the tumor and another with a complex network of blood vessels generated by an MCX simulation. The second version (implemented with both blood distributions) allowed any number of drugs to be conjugated to each antibody. This generalization increases computational time proportional to the number of drug molecules.

The most recent version is a simplification with no blood vessels, where all the drug initially starts on the membrane of a single cell at the tumor's center. This version was built to examine the **bystander effect**, where drug molecules diffuse from one cell to another.

Currently, I am working on expanding these existing simulations to quantify additional values, such as drug concentration in the cytoplasm as a function of distance from the center. I am also comparing different quantities over time.